OAK RIDGE National Laboratory

Oak Ridge Leadership Computing: Science on Summit and Preparing for Frontier

2020 Performance, Portability, and Productivity in HPC Forum
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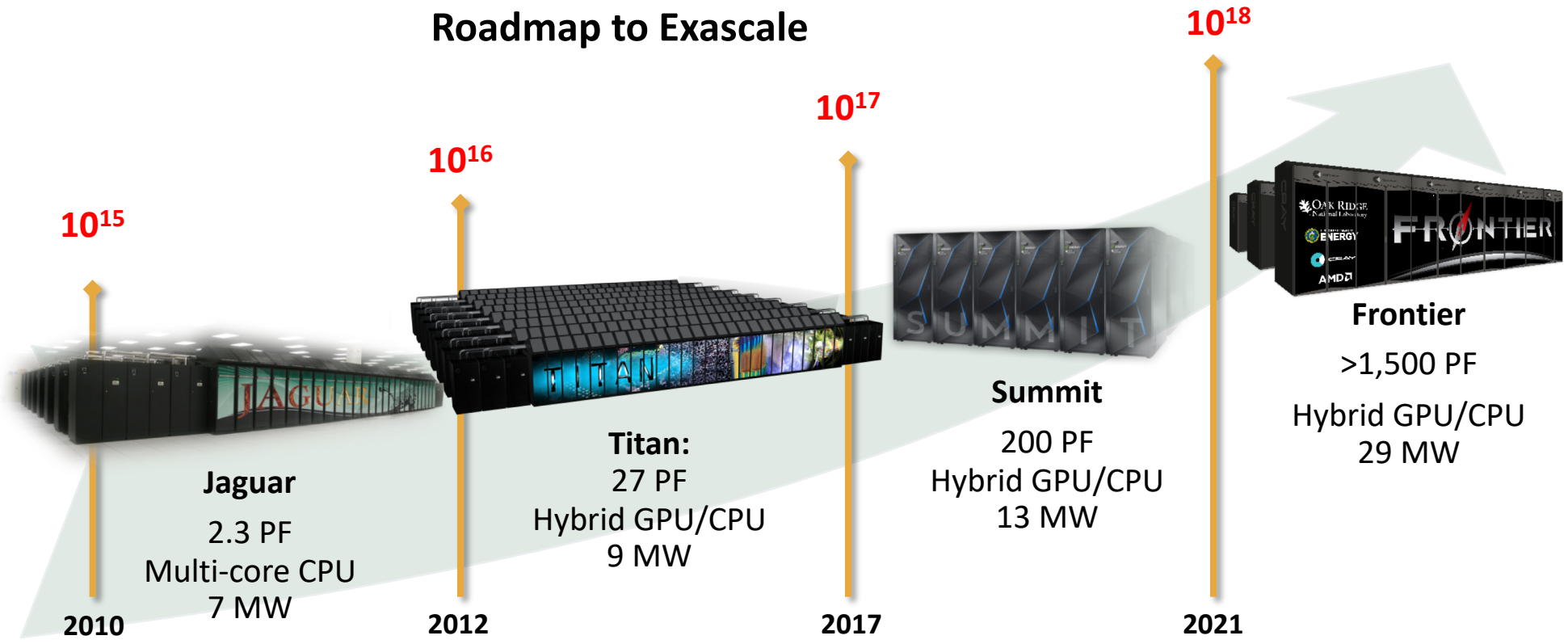
ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

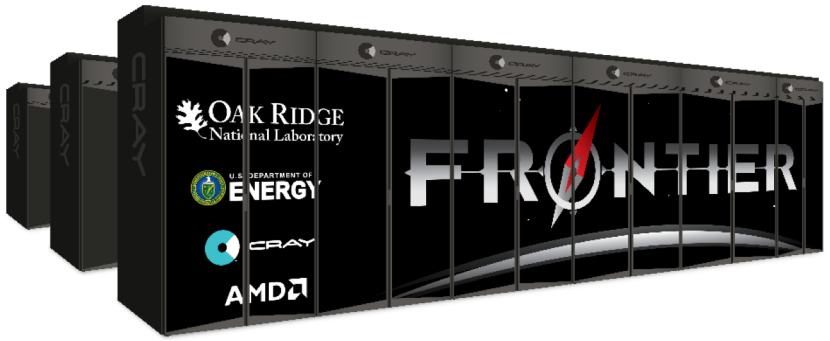
Oak Ridge Leadership Computing Facility – a DOE Office of Science User Facility

Mission: Providing world-class computational resources and specialized services for the most computationally and data intensive global challenges	Vision: Deliver transforming discoveries in energy technologies, materials, biology, environment, health, etc.

Roadmap to Exascale



Frontier Overview



Partnership between ORNL, Cray, and AMD

The Frontier system will be delivered in 2021

Peak Performance greater than 1.5 EF

Composed of more than 100 Cray Shasta cabinets

- Connected by Slingshot™ interconnect with adaptive routing, congestion control, and quality of service

Node Architecture:

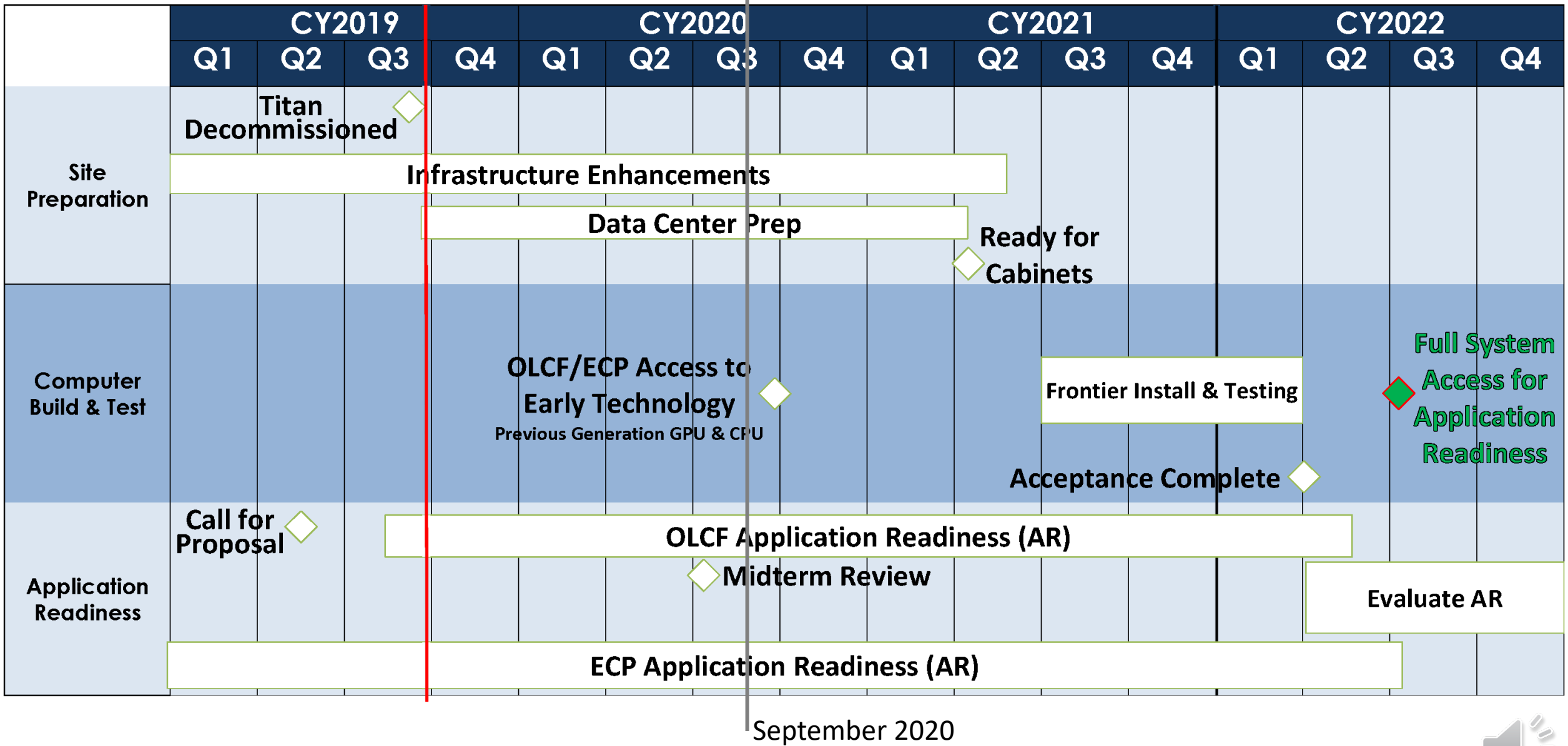
- An AMD EPYC™ processor and four Radeon Instinct™ GPU accelerators purpose-built for exascale computing
- Fully connected with high speed AMD Infinity Fabric links
- Coherent memory across the node
- 100 GB/s injection bandwidth
- Node local NVM storage

Researchers will harness Frontier to advance science in such applications as systems biology, materials science, earth sciences, energy production, additive manufacturing and health data science.

Comparison of Titan, Summit, and Frontier Systems

System Specs	Titan	Summit	Frontier
Peak	27 PF	200 PF	~1.5 EF
# cabinets	200	256	> 100
Node	1 AMD Opteron CPU 1 NVIDIA Kepler GPU	2 IBM POWER9™ CPUs 6 NVIDIA Volta GPUs	1 HPC and AI Optimized AMD EPYC CPU 4 Purpose-Built AMD Radeon Instinct GPU
On-node interconnect	PCI Gen2 No coherence across the node	NVIDIA NVLINK Coherent memory across the node	AMD Infinity Fabric Coherent memory across the node
System Interconnect	Cray Gemini network 6.4 GB/s	Mellanox Dual-port EDR IB network 25 GB/s	Cray four-port Slingshot network 100 GB/s
Topology	3D Torus	Non-blocking Fat Tree	Dragonfly
Storage	32 PB, 1 TB/s, Lustre Filesystem	250 PB, 2.5 TB/s, IBM Spectrum Scale™ with GPFS™	2-4x Summit's performance and capacity, Lustre Filesystem
Near-node NVM (storage)	No	Yes	Yes

Frontier Timeline



Frontier Programming Environment

- To aid in moving applications from Summit to Frontier, ORNL, Cray, and AMD will partner to co-design and develop enhanced GPU programming tools designed for performance, productivity and portability.
- This will include new capabilities in the Cray Programming Environment and AMD's ROCm open compute platform that will be integrated together into the Cray Shasta software stack for Frontier
- In addition, Frontier will support many of the same compilers, programming models, and tools that have been available to OLCF users on both the Titan and Summit supercomputers

Summit is a premier development platform for Frontier

Frontier Portable Programming with HIP

HIP (Heterogeneous-compute Interface for Portability) is an API developed by AMD that allows developers to write portable code to run on AMD or NVIDIA GPUs. It is a wrapper that uses the underlying CUDA™ or ROCm platform that is installed on a system

The API is very similar to CUDA so transitioning existing codes from CUDA to HIP is fairly straightforward.

AMD has developed a “hipify” tool that automatically converts source from CUDA to HIP.

Developers can specialize for the platform to tune for performance or handle unique cases

OLCF has made HIP available on Summit so that users can begin using it prior to its availability on Frontier

Artificial Intelligence and Machine Learning on Frontier

Closely integrating artificial intelligence with data analytics and modeling and simulation will drastically reduce the time to discovery by automatically recognizing patterns in data and guiding simulations beyond the limits of traditional approaches.

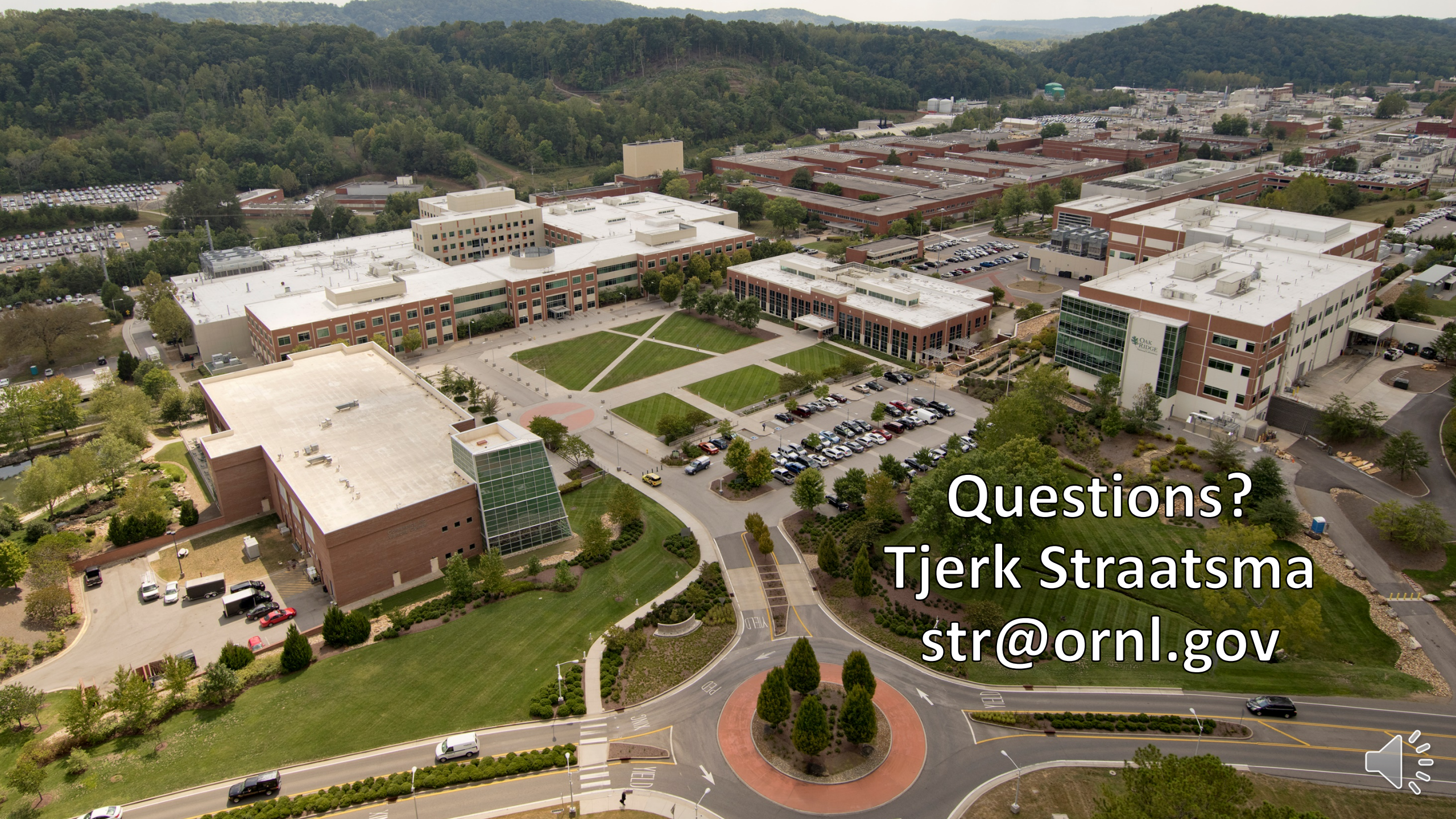
Frontier will have a fully optimized, scalable data science suite in addition to the Cray Programming Environment Deep-learning plugin that provides support for Apache Spark, GraphX, MLib, Alchemist frameworks, and pbdR.

Like Summit, Frontier will be fine tuned to run AI workloads

Application Readiness Efforts for Frontier

Domain	CAAR Project
Astrophysics	CHOLLA
Molecular Dynamics	NAMD
Materials Science	LSMS
Biology	CoMet
Fluid Dynamics	GESTS
Nuclear Physics	NUCCOR
Plasma Physics	PIConGPU
Subsurface Flow	LBPM

Domain	ECP Project
Astrophysics	ExaStar
Cosmology	ExaSky
High Energy Physics	LatticeQCD
Chemistry	NWCHEMeX
Chemistry	GAMESS
Combustion	PELE
Nuclear Energy	ExaSMR
Fusion	WDMApp
Climate	E3SM
Additive Manufacturing	ExaAM
Biology	ExaBiome
Electrical Grids	ExaSGD


Questions?
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